Inferring resource competition in microbial communities from time series

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The competition for resources is a defining feature of microbial communities. In many contexts, from soils to host-associated communities, highly diverse microbes are organized into metabolic groups or guilds with similar resource preferences. The resource preferences of individual taxa that give rise to these guilds are critical for understanding fluxes of resources through the community and the structure of diversity in the system. However, inferring the metabolic capabilities of individual taxa, and their competition with other taxa, within a community is challenging and unresolved. Here we address this gap in knowledge by leveraging dynamic measurements of abundances in communities. We show that simple correlations are often misleading in predicting resource competition. We show that spectral methods such as the cross-power spectral density (CPSD) and coherence that account for time-delayed effects are superior metrics for inferring the structure of resource competition in communities. We first demonstrate this fact on synthetic data generated from consumer-resource models with time-dependent resource availability, where taxa are organized into groups or guilds with similar resource preferences. By applying spectral methods to oceanic plankton time-series data, we demonstrate that these methods detect interaction structures among species with similar genomic sequences. Our results indicate that analyzing temporal data across multiple timescales can reveal the underlying structure of resource competition within communities.

I. INTRODUCTION

The collective biological activity of ecosystems is defined by fluxes of resources. From plant [1] to microbial [2] communities, the availability of resources such as sunlight or reduced carbon and nitrogen enables the generation of energy and the production of biomass. Competition for resources therefore drives ecological interactions between members of the system. As a result, resource-mediated interactions such as competition have long been recognized as central structuring properties of ecosystems across scales.

Perhaps nowhere are the structuring forces of resources more clear than in microbial consortia. Communities of microbes utilize resources in almost every niche on the planet, from carbon remineralization in the photic zone of the ocean [3], to fiber utilization in the rumen of ungulates [4], and the collective transformation of oxidized nitrogen compounds in the soil [5, 6]. In each of these cases, complex communities of hundreds or thousands of species compete for, and utilize, resources to generate energy and biomass.

In these contexts, the metabolic traits of microbes utilizing each resource become a key property of interest because they dictate which species compete for which resources. In part due to the conserved structure of the biochemical pathways that enable the utilization of resources, microbial communities are frequently observed to be comprised of guilds, or groups of species, that utilize a similar set of resources [7, 8]. These guilds, often comprised of tens or more taxa, compete for diverse pools of resources. For example, marine communities utilize complex mixtures of carbon sources [9] and many members of the human gut microbiome utilize mixtures of carbon sources [10]. Thus the mapping of species to the resources they utilize typically has a block-like structure, with groups of species utilizing groups of resources [11].

A second key feature of resource utilization in microbial ecosystems is temporal fluctuations. Temporal variability in resource availability is the norm across many if not most habitats. For example, diurnal fluctuations drive the availability of carbon in photosynthetically driven ecosystems [12], and feeding temporally structures the availability of resources in host-associated microbial communities [13]. Similarly, in soils, transient dynamics in moisture drive large fluctuations in nutrient availability [14].

Given the importance of resources, the central role of microbial traits and temporal fluctuations in mediating the dynamic utilization of resources by communities, a central challenge in the field is understanding resource-mediated interactions in communities. This challenge is highlighted by the fact that in the context of a complex community, we cannot easily access the resources each and every species is utilizing. In most cases, isolating individual strains or taxa and assaying their resource preferences is infeasible. While genome-scale models [15] show potential for predicting resource utilization from sequencing data (shotgun metagenomics) these methods remain highly error-prone for genomes of non-model organisms [16]. In light of these considerations, it is impor-

tant to develop empirically grounded methods to infer the resource-mediated interactions in a complex consortium.

Here, we ask what metrics on the observed time series of species abundances can give us insight into the structure of resource-mediated interactions in the community. In particular, if there are metabolic guilds in the community, how can we reliably infer them from time-series measurements? We approach this problem in the context of consumer-resource models [17]. We focused on consumer-resource formalisms because recent work has shown these models to be powerful quantitative formalisms for understanding abundance and resource dynamics in real communities [6, 18], suggesting that this formalism has some predictive power in the microbial context.

While a host of powerful methods have been developed to infer interactions in ecological communities many of these methods rely on statistical analysis of correlations in species abundances and make simplifying assumptions such as sparsity [19, 20]. Leveraging the widespread availability of time series data in microbial communities [21–23], we present temporal pairwise measurements as novel predictors of resource-mediated species-species interactions and apply them to existing datasets.

II. RESULTS

A. Environment-mediated consumer-resource model

In real experiments, the underlying consumer-resource interactions and resource dynamics are exceedingly challenging to measure. To develop a method that can be applied to analyze experimental time traces, we first introduce a model with known ground truth to develop an appropriate metric, which can reveal the effective resource overlap between species, using only the observed abundances of consumer species.

We consider an ecological system with N species with abundances x_i $(i = 1, \dots N)$ and M resources with concentrations R_α $(\alpha = 1, \dots M)$. Interactions are given by an externally supplied resource model. The dynamical effect of environmental fluctuations is explicitly modeled by the time-dependence of the external supply, $K_\alpha(t)$, that mediates resource availability (Fig. 1(a)) [17, 24–26]. Mathematically,

$$\dot{x}_i = \left(\sum_{\alpha=1}^{M} r_{i\alpha}\gamma_{i\alpha}R_\alpha(t) - d_x \right) x_i(t), \tag{1}$$

$$\dot{R}_\alpha = K_\alpha(t) - \left(d_R + \sum_{i=1}^{N} r_{i\alpha}x_i(t) \right) R_\alpha(t), \tag{2}$$

where $r_{i\alpha}$ is the uptake rate of resource α for species i (and simultaneously the depletion rate of resource α given species i), $\gamma_{i\alpha}$ is the yield of species i given resource α, i.e. how much species i grows by consuming resource α, and d_x and d_R are the death rate of the species and the resources. For simplicity, d_x is set to be equal for all species and d_R across all resources. We call this model the environment-mediated consumer-resource model (ECRM).

Because resources impact species abundances through exponential growth, it will be useful to log-transform species abundances before analysis, denoting

$$\tilde{s}_i(t) \equiv \log x_i(t), \tag{3}$$

which we further normalize as the z-score,

$$s_i(t) = \frac{\tilde{s}_i(t) - \langle \tilde{s}_i \rangle}{\sigma_s}. \tag{4}$$

Intuitively, the z-score describe the deviation from the mean in terms of expected standard deviation.

To model the impact of environment, we assume that its fluctuations directly influence the resource abundance, which then by means of the consumer-resource relation is transmitted through the ecological system. We consider two types of environmental fluctuations, $K_\alpha(t)$.

First, sinusoidal drives are given by

$$K_\alpha(t) = K_\alpha^0 + A_\alpha \sin(\omega_\alpha t - \phi_\alpha), \tag{5}$$

where K_α^0 is the base supply for resource α, A_α the amplitude of the sinusoidal drive, ω_α the frequency, and ϕ_α the phase. This form models the periodic drives omnipresent in nature, for example, diurnal cycles in aquatic systems, or regular food intakes in host-associated microbiomes.

Second, Ornstein-Uhlenbeck (OU) drives evolve according to

$$K_\alpha(t) = K_\alpha^0 + Q_\alpha(t), \tag{6}$$

with K_α^0 the base supply for resource α as in the sinusoidal case and Q_α a stochastic OU process defined by

$$\frac{dQ_\alpha}{dt} = -\omega_\alpha Q_\alpha + A_\alpha \sqrt{\omega_\alpha}\eta_\alpha(t). \tag{7}$$

Here, ω_α and A_α are defined such that both the power and the timescales in the sinusoidal and the OU processes match, and the white noise $\{\eta_\alpha(t)\}$ satisfies

$$\langle \eta_\alpha(t) \rangle = 0, \qquad \langle \eta_\alpha(t)\eta_\beta(t') \rangle = \delta_{\alpha\beta}\delta(t - t'). \tag{8}$$

Compared to sinusoidal drives, OU drives are stochastic, which are useful in modeling environmental fluctuations with unknown strength and regularity such as redox fluctuations in soils [27].

The consumer-resource interaction matrix $\mathbf{C}$, where each entry is $C_{i\alpha} = r_{i\alpha}\gamma_{i\alpha}$, describes the intake of resource α by species i (Fig. 1(b)). Summing over the resources we obtain the resource-utilization overlap matrix $\mathbf{CC}^\intercal$ (Fig. 1(c)). Large off-diagonal entries of this matrix ($\mathbf{CC}^\intercal_{i,j}$) indicate that species i and j have high overlap in the resources they utilize. Species with high resource-overlap are expected to compete, and those without are

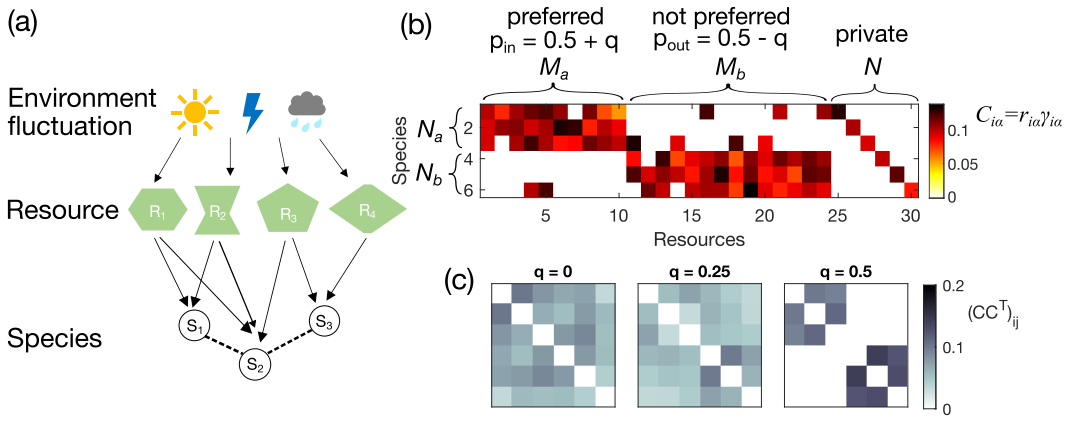

FIG. 1: **Environment-mediated ecological interactions between resources and consumers.** (a) Cartoon of interactions among environment-mediated resources and consumer species. (b) An example of the consumer-resource interaction matrix $\mathbf{C}$ with elements $C_{i\alpha} = r_{i\alpha}\gamma_{i\alpha}$ (colorbar). The probability of non-zero consumer-resource interactions depends on whether the resource is preferred by the species or not, with an adjustable parameter q that encodes guild-structure bias ($q = 0.4$ for this example). All resources also have private resources to prevent extinction. (c) Effective interactions among the species are captured by the effective resource-utilization overlap matrix, $\mathbf{CC}^\intercal$ (colorbar), shown here for 3 different values of the guild-structure bias q.

expected not to compete. One can consider the resource-utilization matrix as a proxy for effective interactions between species, which is informative about the community structure.

Specifically, we are interested in detecting guilds among the interacting species. To introduce a guild structure in resource overlap, we write the uptake rate as $r_{i\alpha} = r g_{i\alpha}$, where $g_{i\alpha}$ is an adjacency matrix that takes the value of 0 if species i does not uptake resource α, and 1 if it does consume this resource. In order to generate ensembles of random interaction strengths such that the resulting $\mathbf{CC}^\intercal$ matrix has a block (guild) structure, we construct a bipartite graph between N species and M resources. We then separate both the species and the resources into k groups, with each group of species preferring to consume resources from one group of resources. The elements of the adjacency matrix that specifies these preferences, $g_{i\alpha}$, are drawn from a Bernoulli distribution parametrized by a probability p_{in}. For the other $k-1$ groups of non-preferred resources, the elements of the adjacency matrix $g_{i\alpha}$ are drawn from a Bernoulli distribution parametrized by a probability $p_{\text{out}} < p_{\text{in}}$. In addition, each species is assigned its private resource to prevent extinction (Fig. 1(b)). The yield $\gamma_{i\alpha}$ is drawn from a Gaussian distribution with a positive mean and small variance to introduce randomness. All yields are non-negative (see **Methods** for specific parameter values).

When there are only two guilds a and b, we can reduce the number of parameters by defining a guild-structure bias q and set $p_{\text{in}} = 0.5 + q$ and $p_{\text{out}} = 0.5 - q$. For the first set of N_a species we set the probability that they consume the M_a resources to $p_{\text{in}} = 0.5 + q$, while their probability to consume the remaining M_b resources is $p_{\text{out}} = 0.5 - q$. The N_b species from the second group have opposite preferences: with probability $p_{\text{out}} = 0.5 - q$ they consume the first M_a resources, and probability $p_{\text{in}} = 0.5 + q$ the remaining M_b resources. Here, q acts as a tuning variable for block structures. If $q = 0.5$, there are zero interactions between species that belong to different guilds. If $q = 0$, there is no bias of any species towards any resource (see Fig. 1(b,c)).

The consumer-resource model (1)-(2), environmental drive (5)-(7), and resource guild structure $r_{i\alpha}$ among consumers, completely define the model. To illustrate its behavior and gain intuition, we first simulated a small network with $N = 6$ species and $M = 30$ resources, with a guild-structure bias of $q = 0.4$. The resource-utilization matrix $\mathbf{CC}^\intercal$ is given by Fig. 2(a). The specific set of parameters is given in Methods IV A. The first $N_a = 3$ species form one guild, while the remaining $N_b = 3$ species form the other. To study the impact of environmental drive on species abundances, we simulate the ECRM under sinusoidal and OU environmental drives each sampled at three different ranges of timescales – slow, fast, and with a mixture of timescales (Fig. 2(b)). Example traces of pairs of species within the same guild show complex coupled dynamics depending on the environmental timescales (Fig. 2(d)).

B. Pairwise measures of species couplings

To explore how the coupled dynamics of species abundances can be informative about their resource overlap $\mathbf{CC}^\intercal$, we consider observables of increasing complexity that measure the deviation from independence between the time traces of two species.

1. *Equal-time correlation* $\mathbf{C}(0)$

We first consider the equal-time correlation coefficient, defined as

$$C_{ij}(0) = \lim_{T\to\infty} \frac{1}{T} \int_0^T s_i(t)s_j(t)dt, \tag{9}$$

which for finite data time-series size sampled at a finite sampling rate is

$$C_{ij}(0) \approx \frac{1}{T} \sum_{t=1}^{T} s_i(t)s_j(t), \tag{10}$$

where $t = 1, \ldots, T$ now denotes the time frame. As equal-time correlations describes how much the concentrations of pairs of species fluctuate together, it is a measure commonly used in detecting species-species interactions. However, it is known that equal-time correlations cannot accurately reproduce the interactions [20].

Specifically, as shown in Figure 2(c) in our example of 6 species distributed into 2 guilds, when the environmental drive is fast, $C_{ij}(0) \propto (\mathbf{CC}^\intercal)_{ij}$, while when the environmental drive is slow, $C_{ij}(0) \propto -(\mathbf{CC}^\intercal)_{ij}$. Intuitively this happens because fast resource dynamics drive coherent responses of members within a guild, but slow resource dynamics lead to competition within guilds (the underlying mechanism is first explored and explained in detail in [28]). This problem is more pronounced when environmental fluctuations are driven by a mixture of timescales (middle panel in Fig. 2(c)). There is no correlation between the equal-time correlation $\mathbf{C}(0)$ and the resource utlization overlap $\mathbf{CC}^\intercal$ (p-value = 0.4, Spearman correlation test). In this example, the pair of species with the strongest resource utlization overlap (indicated by red boxes in Fig. 2(a)) has a equal-time correlation close to 0, as indicated by the black arrow in Fig. 2(c).

Without knowing *a priori* the timescale of the environmental fluctuation, the equal-time correlation $\mathbf{C}(0)$ does not return a good enough estimator of the resource utlization overlap.

2. *Cross-correlation with time-delay reveals species interaction structure*

Since equal-time correlations do not reveal the stucture of effective species-species interactions, we took a closer look at time series data. Let us focus again on the pair of species with the strongest resource overlap (red box in Fig. 2(a)). As shown by Fig. 2(d), the time evolution of species abundances depends heavily on the environmental drive. Under fast environmental drive, the two species abundances track each other closely, while under slow drive, they exhibit a phase shift. When the environmental drive is mixed with fast and slow modes, the dynamics of each species also exhibit a mixture of modes, and the relation between the two species is less clear.

Given a complicated time-series, we need to consider dynamical pairwise measures, such as the time-delayed cross-correlation function,

$$C_{ij}(\tau) = \lim_{T\to\infty} \frac{1}{T} \int_0^T s_i(t)s_j(t+\tau)dt. \tag{11}$$

As shown in Figure 2(e), under all three types of environmental drive, the absolute value of the cross-correlation at certain time lags is large, which suggests that it carries information about the species–species interaction structure. However, if one only considers a single time delay, e.g. $\tau = 0$, the value can be very close to 0.

Comparing across different pairs of species, we observe that the cross-correlation function between species of the same guild varies with a much larger amplitude than between species from a different guild (Fig. 3(a) *left panel*, pairs of distinct species belonging to the same guild are outlined in red). However, different pairs of interacting species show signatures of strong cross-correlations at different time delays τ, implying that there is no *a priori* choice of any single time delay that would reveal the interaction structure between all pairs of species.

3. *Spectral method for time-series analysis: Cross power spectral density (CPSD) and coherence*

In order to focus on the interplay of timescales, we reformulated the dynamical pairwise measures in the frequency domain. Spectral analysis has been used to probe many aspects of ecological systems [29]. Here, we measure the cross power spectral density (CPSD) by taking the Fourier transform of the cross-correlation function,

$$P_{ij}(f) = \int_{-\infty}^{\infty} C_{ij}(\tau)e^{-i2\pi f\tau}d\tau. \tag{12}$$

We divide its magnitude-squared by the power spectral density of each of the two time series, to define the (magnitude-squared) coherence,

$$\mathrm{Coh}_{ij}(f) = \frac{|P_{ij}(f)|^2}{P_{ii}(f)P_{jj}(f)}. \tag{13}$$

Coherence ranges between 0, when the two signals are unrelated, and 1, when they are perfectly correlated up to a phase shift. It is used in signal processing to detect relations between two signals [30].

Figure 3(a) shows a schematic of how to compute CPSD and coherence from the cross-correlation function for the example network in Fig. 2(a) with mixed timescales of the environmental drive. Recalling that the underlying resource utlization overlap network has a block structure (the first three species belong to the same guild, and the last three species belong to another guild), it becomes clear from Fig. 3(a) that both the magnitude of the CPSD and the coherence are larger between intra-guild pairs of species than between inter-guild species. As

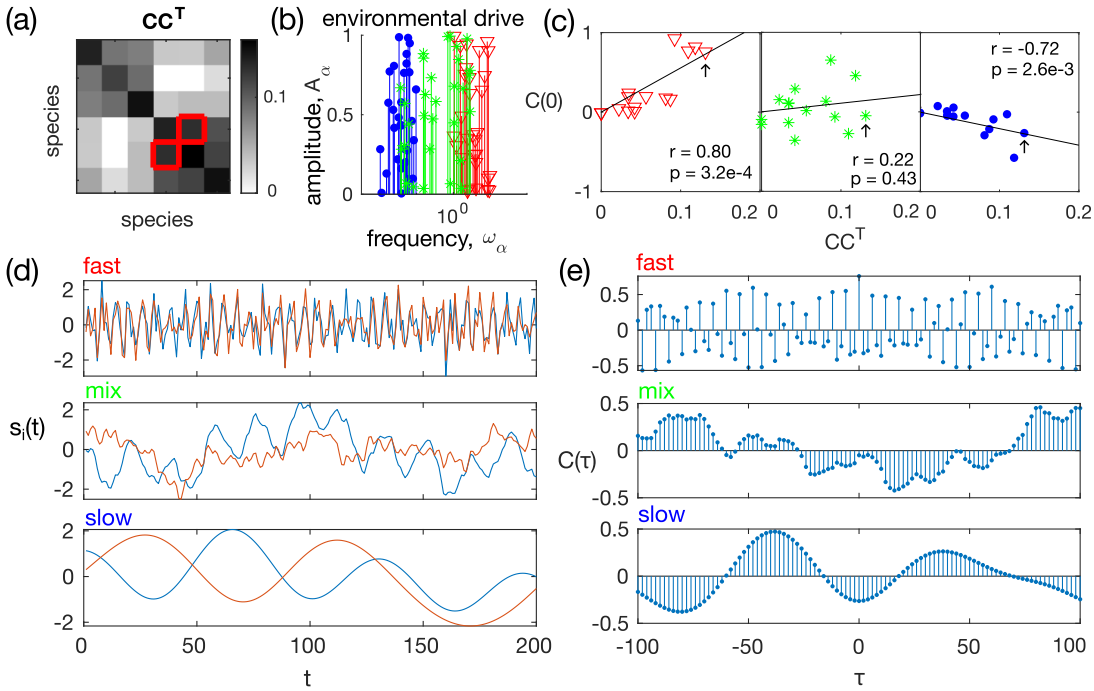

FIG. 2: **The simulated guild based ecosystem.** An example environment-mediated consumer-resource model (number of species $N = 6$, number of resources $M = 30$, and guild-structure bias $q = 0.4$) demonstrating that the relation between the equal-time species abundance correlation $\mathbf{C}(0)$ and the underlying resource utilization overlap matrix $\mathbf{CC}^\intercal$ depend on the timescale of the environmental drive. (a) Resource utilization overlap matrix $\mathbf{CC}^\intercal$. The red boxes indicate an example pair of interacting species. (b) Environmental drives are chosen to be sinusoidal, with fast (*red*, $\omega_\alpha \in [1, 10]$), slow (*blue*, $\omega_\alpha \in [0.01, 0.1]$), and mixed timescales (*green*, $\omega_\alpha \in [0.03, 3]$). (c) The correlation between the elements of equal-time correlation function $\mathbf{C}(0)$ and the elements of the resource-utilization matrix, $\mathbf{CC}^\intercal$, is positive when the environmental drive is fast (*red*); negative when the drive is slow (*blue*), and shows no correlation when the drive is composed of a mixture of slow and fast timescales (*green*). In each panel, r is Spearman's rank correlation coefficient, p is the p-value for the null hypothesis that there is no correlation between $\mathbf{C}(0)$ and $\mathbf{CC}^\intercal$. Black arrows indicate the example pair of species in the red boxes of (*a*). (d) Example segments of time series of the log-transformed species abundances for the red-boxed pair of (*a*), under the three types of environmental drive given in panel (*b*). (e) Cross-correlation function between the species abundances of the example red-boxed pair of (*a*). Equal-time correlation is the value of $\mathbf{C}(\tau)$ at $\tau = 0$.

coherence further reduces the impact of individual species (due to normalization), the difference between intra- and inter-guild pairs is larger in the coherence than in the CPSD magnitude (Fig. 2(a)).

Both CPSD and coherence are frequency dependent and contain information about the relation between the species abundance z-scores $s_i(t)$ and $s_j(t)$ at each frequency. To obtain an aggregate measure of the coupling between species abundances over many timescales, we consider the integral of the CPSD magnitude and coherence across all frequencies. Specifically,

$$\mathcal{P} \equiv \int_0^{f_{\max}} |P_{ij}(f)| df \approx \sum_{k=0}^{k_{\max}} |P_{ij}(f_k)| \Delta f, \qquad (14)$$

where Δf is the frequency resolution we choose when performing the discrete Fourier transform. Note that if we integrated the CPSD without taking its magnitude, we would recover the equal-time correlation by Parseval's theorem.

Likewise, we define the total coherence as the integral of the magnitude squared coherence across all frequencies,

$$\mathcal{TC}_{ij} \equiv \int_0^{f_{\max}} \mathrm{Coh}_{ij}(f) df \approx \sum_{k=0}^{k_{\max}} \mathrm{Coh}_{ij}(f_k) \Delta f. \qquad (15)$$

The maximum frequency is given by the Nyquist frequency, $f_{\max} = 1/2\Delta t_{\text{sampling}}$. The frequency resolution Δf is chosen heuristically, such that the power spectral density estimate is relatively stable when Δf is doubled or halved ($\Delta f = f_{\max}/15$ for all the results presented in this manuscript). Using the simulated ECRM data, we estimate the power spectral density of the species abundance time series using the MVGC Toolbox [31] and the MATLAB built-in function with Welch's method to reduce noise from using finite data. As shown in Fig. 3(b), compared to the equal-time correlation $\mathbf{C}(0)$ and its absolute value, both the total magnitude of CPSD $\mathcal{P}$ and the total coherence $\mathcal{TC}$ are much more informative of the underlying resource utilization overlap matrix $\mathbf{CC}^\intercal$. Total coherence is the best of the four predictors. This ad-

vantage of the total coherence persists for both ECRMs under sinusoidal and OU drives and over the range of guild-structure biases q (Fig. 3(c)).

Thus, the two proposed measures $\mathcal{P}$ and $\mathcal{TC}$ offer a proxy for the resource-overlap interactions between species.

C. Binary classifier for guild-structure detection

In many cases, one is interested in recovering the guild structure of the community from time series [32]. Identification of guild structure can enable a massive dimensional reduction in the dynamic description of the system and provide insight into key metabolic properties [33].

Motivated by this, we asked whether total coherence and CPSD magnitude could be used to learn the large-scale guild structure of $\mathbf{CC}^\intercal$. We used the four pairwise measures, $\mathbf{C}(0)$, $|\mathbf{C}(0)|$, $\mathcal{P}$, $\mathcal{TC}$, as scores to perform a binary classification between pairs of species belonging to the same guild and pairs belonging to different guilds. We applied this approach to our small $N = 6$ simulated ECRM system with 2 guilds (Fig. 2(a)). To obtain a consistent partition into guilds, we perform single linkage clustering initiated from all pairs of species whose pairwise measure is larger than a threshold within the range of the pairwise measure. For example, if after thresholding species i and j are determined to belong to the same guild, as well as species j and k, then all three species i, j, k are grouped into to the same guild.

To visualize the performance of the binary classifiers, we plot the Receiver Operator Curve (ROC) across different thresholds (Fig. 4(a)). The total coherence outperforms all other measures in correctly partitioning species into guilds. The Area Under the ROC (AUC) shows the advantage of coherence persists for all guild biases q (Fig. 4(b)). For $q = 0$ there is is no guild structure to detect and all measures fail at the task, as they should. The ROC and AUC of the equal-time correlation predictor $C_{ij}(0)$ shows that it performs only slightly better than random guessing (AUC = 0.5), for all values of q. Taking its absolute value improves prediction beyond random guessing, but is still worse than the spectral measures $\mathcal{P}$ and $\mathcal{TC}$.

D. Spectral methods work for general ECRM systems with larger sizes

In natural ecological systems, both the number of guilds and the number of species in each guild can be large. How well can the dynamical pairwise observables predict the resource utlization overlap for different system sizes? We now consider general ECRMs with larger number of guilds. To explore finite size scaling, we consider three families of ECRMs with numbers of species, resources, and guilds given in Table 1.

N	$M \propto N$	$k \propto \sqrt{N}$
6	30	2
24	120	4
96	480	8

TABLE 1: Parameters for the ECRM with different system size.

As we increase the size of the ECRMs by increasing the species size N, we also increase the number of resources in proportion, $M \propto N$, and the number of guilds as $k \propto \sqrt{N}$. We take $p_{\text{in}} = (1/2 + q)\,(N/6)^{-1/2}$ and $p_{\text{out}} = (1/2 - q)\,(N/6)^{-1}$. The scalings with N are chosen such that the average connectivity degree for each species in the effective resource-utilization matrix $\mathbf{CC}^\intercal$ becomes constant at large N (see **Methods** IV B for details). The particular prefactors are chosen so that the numbers are consistent with the $N = 6$ case considered earlier.

We monitor the predictive performance of the same four pairwise measures as before ($\mathbf{C}(0)$, $|\mathbf{C}(0)|$, $\mathcal{P}$, and $\mathcal{TC}$) as we increase the system size from $N = 6, k = 2$ to $N = 24, k = 4$, and then to $N = 96, k = 8$ (Fig. 5(a,e,i)). We compute Spearman's correlation coefficient between the pairwise observables and the elements of the $\mathbf{CC}^\intercal$ matrix (Fig. 5(b, f, j)), and the ROC of guild detection after single linkage clustering (Fig. 5(d,h,i)).

By the choice of scaling for p_{in} and p_{out}, the $\mathbf{CC}^\intercal$ matrix is sparse for all system sizes. We can set a threshold on our measures to perform link detection, i.e. identify whether there exists an effective interaction between species due to competition for the same resource. As shown in Fig. 5 for $q = 0.5$ (and SI Fig. S1 for $q = 0.4$), for all the three system sizes tested, the total coherence remains the best among the four predictors. The summary statistics in Fig. S2 show that the total coherence always performs the best among the four predictors, although all get worse as the system size increases. Guild detection (Fig. S2(c)) has a better AUC than link detection (Fig. S2(b)), especially for large system sizes, thanks to error correction afforded by single-linkage clustering.

E. Reconstruction of the $\mathbf{CC}^\intercal$ matrix depends on sampling rate and total time series length

The success of CPSD and coherence in detecting guild structures depends on the interplay of multiple timescales. These timescales include the doubling timescale $(\gamma r)^{-1}$ of the species, their typical lifetime d_x^{-1}, the environmental fluctuation timescales ω_α^{-1}, and their relaxation time d_R^{-1}. Additionally, there are experimental timescales: the total time t_f of data acquisition and sampling interval $\Delta t_{\text{sampling}}$. Here, we discuss the effects of the finite time series and sampling rate on recovering the elements and structure of the $\mathbf{CC}^\intercal$ matrix.

As we increase the total time of acquisition t_f, the ac-

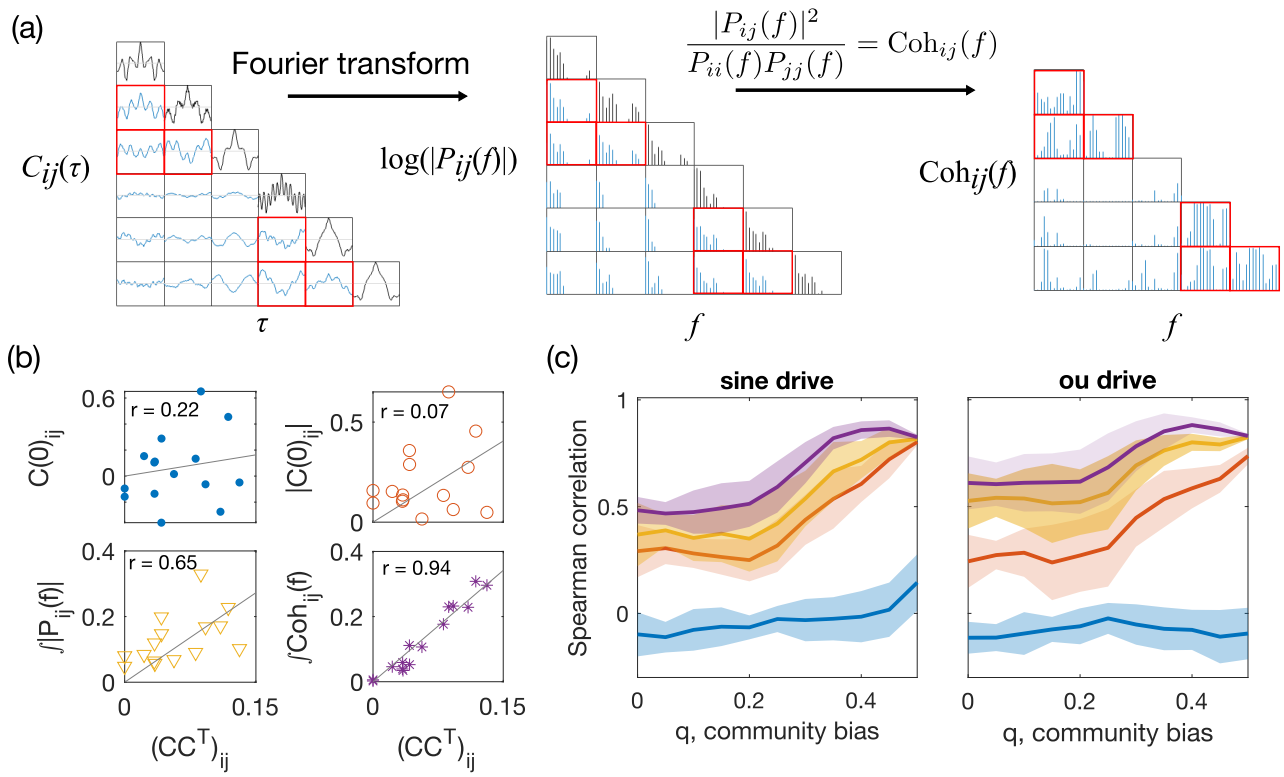

FIG. 3: **Dynamical pairwise observables reveal more about the resource utlization overlap structure than equal-time correlations.** (a) A schematic representation for calculating dynamical observables from the cross-correlation function. The pairwise cross-correlation function (left) is Fourier-transformed into the cross power spectral density (CPSD) (middle), and squared and normalized to obtained the squared coherence (right). All plots show results for the ECRM example in Fig. 2 under an environmental drive with mixed timescales. Pairs of species within the same guild are indicated by red boxes. The guild-structure bias is $q = 0.4$. (b) Scatter plots between pairwise observables for each pair of species and the elements of the effective resource-utilization matrix $\mathbf{CC}^\intercal$ for same data as in panel (a). Pairwise observables include the equal time correlation $\mathbf{C}(0)$ (reproduced from Fig. 2(b) *middle panel*), its absolute value $|\mathbf{C}(0)|$, the total magnitude of CPSD ($\mathcal{P}_{ij} = \int df |P_{ij}(f)|$), and the total coherence ($\mathcal{TC}_{ij} = \int df \mathrm{Coh}_{ij}(f)$). r is the Spearman's rank correlation coefficient. (c) Prediction performance of the pairwise measures of species abundance for resource utlization overlap, given by Spearman's correlation coefficient between the measure and the resource-utilization matrix value, as a function of the guild-structure bias q (same color code as panel (*b*)). Shaded areas represent standard deviation across 10 realizations of the network, each with 10 random realizations of environmental drive given by a sinusoidal process with ω_α sampled log-uniformly $\in [0.03, 3]$ (*left*), or by an OU process with $\omega_\alpha = 1$ (*right*). The total duration of the simulated trajectory is $t_f = 20000$. The sampling timestep is $\Delta t_{\mathrm{sampling}} = 1$.

curacy of guild detection improves for all 4 observables as measured by AUC, as expected (Fig. 6(a)-(d)). For equal-time measurements ($\mathbf{C}(0)$ and $|\mathbf{C}(0)|$, (Fig. 6(a), (b)), the sampling interval $\Delta t_{\mathrm{sampling}}$ does not change the prediction significantly. However, for the total absolute CPSD and the total coherence (Fig. 6(c), (d)), the AUC for guild detection shows an optimal near $\Delta t_{\mathrm{sampling}} = 2$ and $\Delta t_{\mathrm{sampling}} = 0.5$ respectively, for which the AUC for guild detection is largest for the biggest range of total data acquisition timescale. For comparison, in our simulation the species death rate is $d_x = 0.3$, corresponding to a turnover timescale of 3. In the limit of small t_f and large $\Delta t_{\mathrm{sampling}}$, the number of time points is less than the number of the time points required by spectral method given the frequency resolution we specified (for FFT the number of data points needs to be at least double the number of the frequency resolution), which means the methods cannot work (bottom right corner of Fig. 6(d)). Similar results hold for Spearman's correlation between the pairwise metrics and the $\mathbf{CC}^\intercal$ matrix element (SI Fig. S3).

In summary, predictions always benefit from longer time traces, but there exists an optimal, finite sampling frequency for the two spectral methods, which perform best.

F. Reconstructing guild structure from relative species abundances

When dealing with genomic data, often only relative abundances of the species rather than absolute abundances are available. We tested whether the CPSD and coherence observables remain useful for species structure

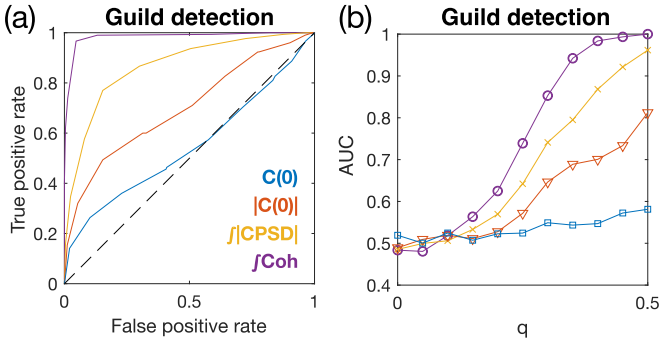

FIG. 4: **Guild detection of resource utilization overlap using the pairwise measures of species abundances with single linkage clustering.** (a) Receiver Operator Curve (ROC) for successfully distinguishing same-guild from different-guild pairs of species using the 4 pairwise measures, from 50 random realizations of the simulated model in Fig. 2. The guild-structure bias is set to $q = 0.4$. (b) Area under the ROC (AUC) for guild detection. Same color code as (a). Environmental drives are given by OU processes with $\omega_\alpha = 1$. Total duration is $t_f = 20000$. Sampling time step $\Delta t_{\text{sampling}} = 1$.

inference from relative abundances, for systems of different sizes.

SI Fig. S4 shows that, for small number of species ($N = 6$ and 24), total coherence has poor predictive power when using relative abundances, while the total magnitude of CPSD still performs well. This result is surprising since coherence as a function of frequency has more structure than CPSD. However, total coherence outperforms other measures for large numbers of species ($N = 96$). This result is consistent with previous work [20] where the impact of relative abundance was reported to be less severe when the number of species is large.

G. Applying temporal metrics to marine data

To illustrate the usefulness of CPSD and coherence on real data, we tested our 4 pairwise metrics on a public dataset consisting of time-series of relative abundance of a total of 49,637 bacterial and eukaryotic operational taxonomic units (OTUs) from coastal plankton collected over 93 consecutive days [22]. For each of the 93 days we have 3 samples for each OTU, and we use the averaged relative abundance across the 3 samples as the relative abundance for each OTU. As the spectral methods have so far been developed considering consecutive time points sampled at regular intervals, we choose to analyze only the eukaryotic OTUs, because the bacterial data contained missing days across all OTUs. Furthermore, since our methods have been developed and tested on synthetic data without zero abundances, we limit our analysis to the $N = 31$ eukaryotic OTUs which are present on each of the 93 days. As the total number of eukaryotic OTUs is much larger than the considered subset, we expect the total coherence and the total magnitude of CPSD should not be adversely effected by the use of relative abundances.

We use the time series of the relative abundances of the $N = 31$ eukaryotic OTUs to compute the four pairwise metrics as described in the previous sections: the equal-time correlation $\mathbf{C}(0)$ its absolute value $|\mathbf{C}(0)|$, the total magnitude of CPSD $\mathcal{P}$, and the total coherence $\mathcal{TC}$. Ideally, we would like to compare the pairwise metrics with the elements of the resource utilization overlap matrix $\mathbf{CC}^\intercal$. However, since there is no *a priori* measurement or knowledge of the guild structure in natural communities, we use phylogenetic distance as a proxy, following previous work [34]. The intuition is that the closer the species are genetically, the more likely they are to share the resources [35].

Comparing the pairwise metrics of the species abundances and the pairwise phylogenetic distance (Fig. 7(a)), all four pairwise metrics exhibit a weak negative correlation with the phylogenetic distance, indicating that more closely related taxa are more likely to share resource utilization capabilities, which is consistent with the literature [34, 36]. After binning the phylogenetic distances using regular intervals and computing the mean and average of the pairwise metrics in each bin, the trend in negative correlations becomes more visible (Fig. 7(b), *colored bars*). To examine whether this negative correlation is statistically significant, we created a null model by destroying any phylogenetic correlation by randomly shuffling the indices of the time series before computing the pairwise metrics. The randomization is performed 10^5 times to collect statistics. As shown by the gray error bars in Fig. 7(b), the null model results in flat pairwise metrics for all metrics, as a function of the phylogenetic distance. At large phylogenetic distances, the data and the index-shuffled null model return the same mean and variance, as indicated by the overlaying errorbars in Fig. 7(b).

Among the four metrics, total coherence exhibits the biggest difference between the data and the null model for small phylogenetic distances, with a p-value of 5×10^{-5} for the test of the mean in the first bin against the index-shuffled null model (see **Methods** IV D for details). These results indicate that even for data collected experimentally in nature, total coherence works well in distinguishing structures in OTUs sharing common resources.

With the pairwise metrics, now we can infer guild structures among the $N = 31$ eukaryotic OTUs using single-linkage clustering with a tunable threshold on the metrics(SI Fig. S5(a)). As there is no *a priori* knowledge of how those eukaryotic OTUs share resources, i.e. no ground truth to compare the guild structure to, we take the strategy of comparing the inferred structures across the four pairwise metrics. The threshold for each metric is selected such that the resulting number of clusters, including singletons, is the same for all four pairwise met-

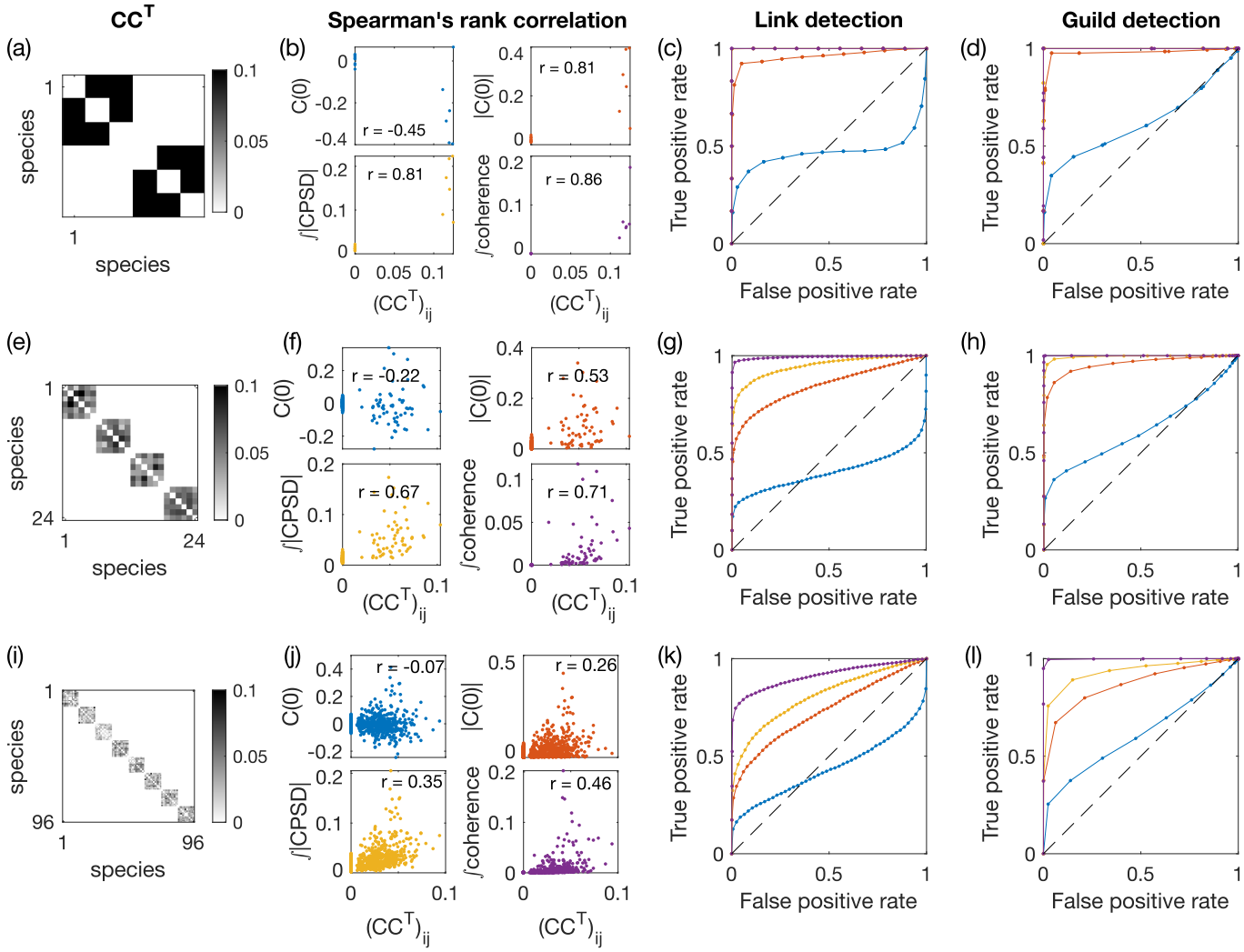

FIG. 5: **Pairwise observables for the simulated ECRM ecosystem of different sizes** (Table 1), with $q = 0.5$. (a) Effective resource-utilization matrix $\mathbf{CC}^\intercal$ with $N = 6$ species, $M = 30$ resources, $k = 2$ guilds, and $q = 0.5$. (b) Correlation between pairwise measures of the species abundances and the resource utilization overlap. Measured pairwise observables include equal-time correlation $\mathbf{C}(0)$ and its absolute value $|\mathbf{C}(0)|$, the total absolute value of CPSD, and the total coherence. (c) ROC curve of link detection for the four pairwise observables. Same color code as panel (b); note that the total absolute value of CPSD overlaps with the total coherence, as both measures return perfect predictions. (d) Same as (c) but for guild detection, after performing single linkage clustering on the pairwise metrics with a tunable threshold. (e-h) Same as (a-d) but for $N = 24$, $M = 120$, and $k = 4$. (i-l) Same as (a-d) but for $N = 96$, $M = 480$, and $k = 8$. For all ECRMs, the environment is driven by OU processes with the intrinsic timescale set to $\omega_\alpha = 1$. For all system sizes, the total duration of the simulated trajectory is set to $t_f = 20000$, and the sampling timestep is set to $\Delta t_{\text{sampling}} = 1$.

rics ($k = 13$). The thresholded connections can be found in SI Fig. S5(b).

As shown by Fig. 7(c), different metrics yield different predicted community structures. Clustering based on coherence gives two non-trivial clusters that exclusively contain OTUs of the same class, which does not occur for other metrics. The equal-time correlation $\mathbf{C}(0)$ and its absolute value $|\mathbf{C}(0)|$ return similar networks. Meanwhile, the total absolute CPSD gives a different network with one giant component and many singletons. This further suggests that the coherence metrics provides a useful predictor of species functional relationships.

III. DISCUSSION

We have shown that by judicious analysis of abundance dynamics data, one can reliably learn patterns of resource competition in microbial communities. Our success emerged from three key perspectives that distinguish this study from prior work.

First, rather than attempting to infer effective interactions between taxa such as those described by a Lotka-Volterra framework [37], we focus on resource-mediated interactions. Consumer resource models have been shown to quantitatively predict abundance and resource dynam-

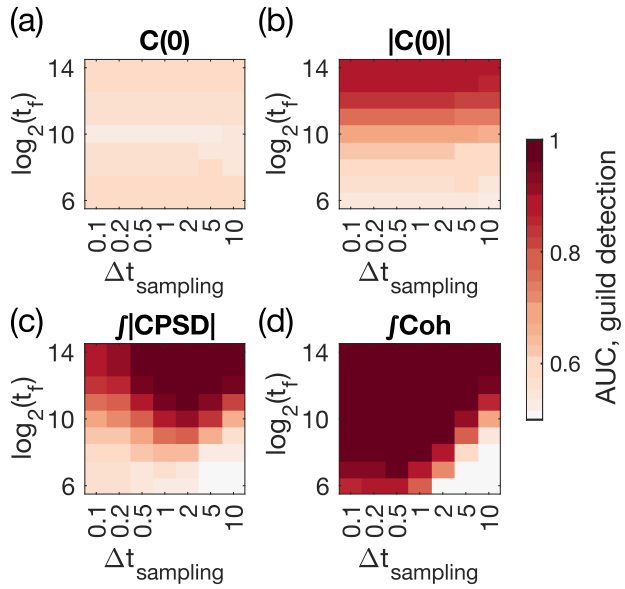

FIG. 6: **Influence of finite data duration and sampling rate on guild detection using pairwise measures of species abundance.** AUC of the guild detection task using (a) Equal-time correlation $\mathbf{C}(0)$, (b) its absolute value $|\mathbf{C}(0)|$, (c) the total absolute value of CPSD, and (d) the total coherence, as the function of sampling duration t_f and interval $\Delta t_{\text{sampling}}$. For reference the species turnover timescale is $d_x^{-1} = 3.33$. The ECRM is the same as the one considered in Fig. 3 with $N = 6$, with OU environmental drive at $\omega_\alpha = 1$ and guild-structure bias $q = 0.4$.

ics in communities [6, 18]. Further, resource-explicit formalisms do not suffer from the ambiguities of effective interactions, especially in the context of microbial communities [38]. Moreover, the resource-centric picture of communities naturally motivates us to focus on coarse patterns of resource utilization overlap, which are empirically supported by the existence of guilds in communities. Guilds allow us to simplify the problem from trying to infer every interaction in a community to inferring a lower-dimensional structure that aggregates strains together by resource preferences.

Within this dynamic resource-centric picture, our second key innovation was to move beyond simple correlations ($\mathbf{C}(0)$) by employing spectral methods that utilize full temporal information. Our method stands in contrast to covariance-based approaches [19, 20] that estimate covariance or inverse covariance matrices to infer associations but do not utilize dynamics. One exception is a recent study that employs temporal delays and Granger causality to infer associations [39]. Similarly, spectral metrics (CPSD and coherence) provide a high-fidelity picture of resource overlaps in communities by extracting information from multiple temporal delays. We expect these methods will prove powerful for inferring structure in complex communities where the acquisition of high-resolution time series has become commonplace.

Finally, our spectral methods not only embrace but rely on the inherently dynamic nature of the environment ($R_\alpha(t)$). In contrast, time-series methods, including those based on Lotka-Volterra (LV) models [40], often assume steady-state dynamics [41, 42] (with notable exceptions [24, 25]). However, it is empirically clear that microbes live in environments that are inherently dynamic [14]. One of the most striking pieces of evidence of the importance of resource dynamics in the microbial world is recent physiological work showing that bacteria dynamically allocate cellular resources in a manner that optimizes growth under changing environments but not steady state conditions [43, 44]. Therefore, we regard the fact that our method relies on resource-driven abundance dynamics as an empirically motivated strength.

Using this approach, our analysis of eukaryotic microbial dynamics in a high-resolution marine dataset showed promising results in two domains. First, we observed that spectral methods outperform simple correlations in detecting statistically significant resource overlap between phylogenetically related taxa (Fig. 7B). Second, it is enticing that these methods yield distinct network architectures from the same data (Fig. 7C). An important avenue for future work is to more carefully vet the predicted associations from these metrics with synthetic communities.

Despite these successes, there are important avenues for improvement. First, as discussed above, at present, our method does not naturally deal with missing time points, uneven temporal sampling, or zeros in the data. It is an important avenue for future work to merge these methods with recent principled advances for handling zeros in amplicon sequencing data [45] or utilizing Lomb-Scargle periodogram methods for unevenly sampled data [46].

Finally, our work complements recent efforts to infer consumer-resource models or metabolic parameters directly from sequencing and metabolomic data [6, 16, 47]. The method of Goyal *et al.* [47] attempts to infer a much more detailed resource-exchange network by using genomic and metabolomic data to pinpoint actual cross-feeding interactions. An exciting avenue for future work would be to combine the sophisticated spectral methods developed here with more explicit genomic or metabolomic datasets.

IV. METHODS

A. Initialize parameters of ECRMs

For all system sizes, the parameters of the ECRM systems are set as the following. The uptake rate for non-zero resource intake is set to $r = 0.1$. The yield $\gamma_{i\alpha}$ is given drawn from a Gaussian distribution with mean 1 and standard deviation 1/6. Redraws are performed to ensure all yields are non-negative. Death rate of the species is set to $d_x = 0.3$, while depletion rate of the resource is set to $d_R = 0.5$. For sinusoidal drives, the timescales of the environmental fluctuation, ω_α, are cho-

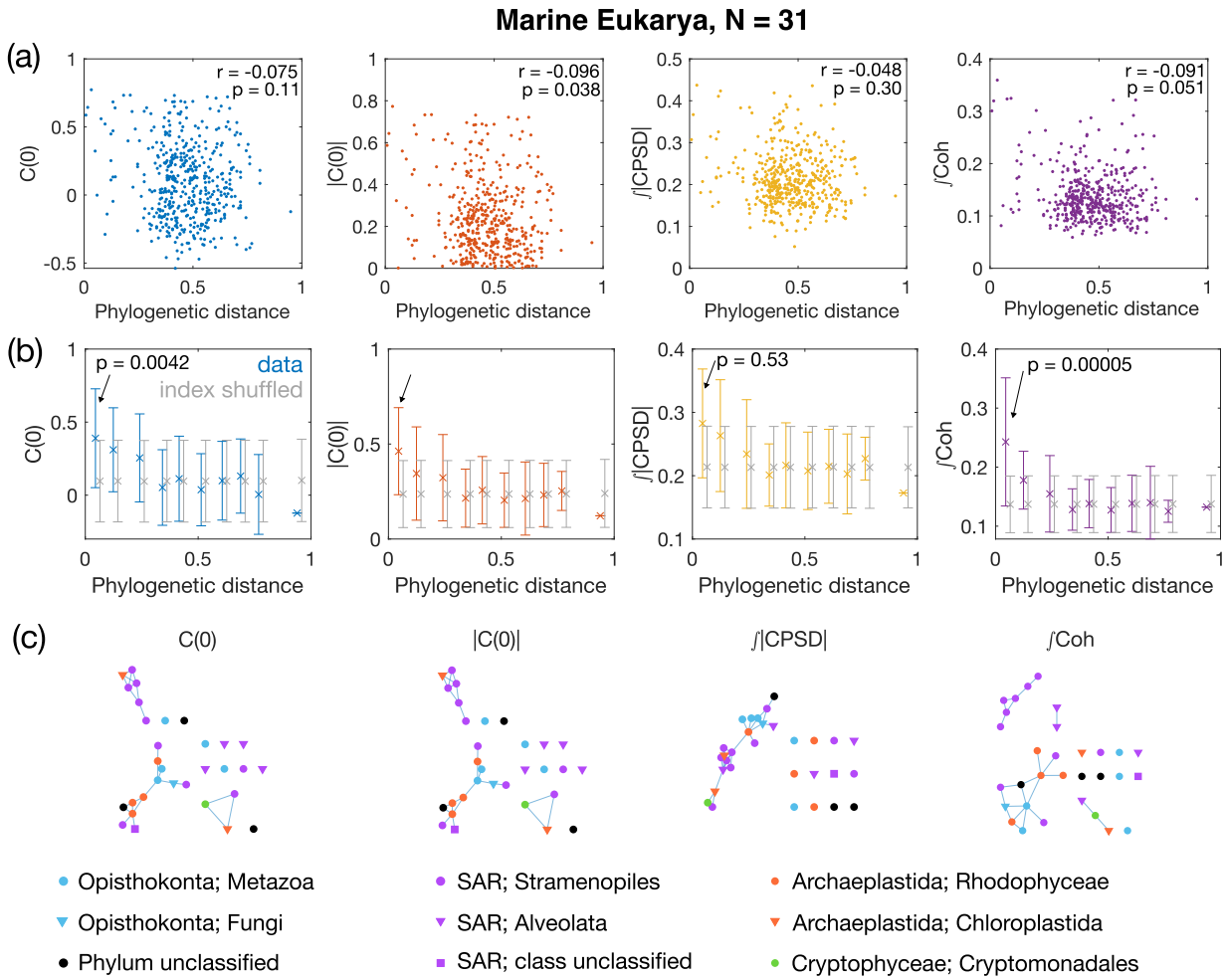

FIG. 7: **Pairwise metrics of the relative abundances of marine eukaryotic OTUs correlate with phylogeny.** (a) Scatterplot of pairwise metrics of relative abundance exhibit a weak anti-correlation with the pairwise sequence distance (Jukes-Cantor distance). Data are from [22] (downsampled to $N = 31$, see text). Pairwise measures include the equal-time correlation $\mathbf{C}(0)$ and its absolute value $|\mathbf{C}(0)|$, the total magnitude of CPSD, and total coherence. Spearman's rank correlation coefficient r and the p-value are given in each panel. (b) Binned average of the pairwise metrics vs. pairwise sequence distances. Binning is taken at regular intervals of the sequence distance. The mean across each bin is plotted with a cross symbol, and error bars given the standard deviation within each bin. In grey are shown the results from a randomized control, where the order of indices of eukaryotic OTUs are shuffled randomly (number of shuffling $= 10^5$). The p-value for the mean of the pairwise metrics in the first bin to be different from the index shuffled null model is given in each panel (see **Methods** IV D for details). (c) Resource overlap networks inferred using the four pairwise metrics, with threshold set to produce $k = 13$ clusters including singletons. The phylum and class of each OTU is given by respectively the color and the shape of the node, and in the legend with the format *phylum*;*class*.

sen randomly from a log-uniform distribution with a predetermined range to represent the mixture of multiple timescales in real environment and to avoid resonance. The phase ϕ_α is chosen from a uniform random distribution between 0 and 2π. For OU environmental drives, thanks to its stochastic nature, we can choose the intrinsic frequencies ω_α to be the same for all resources α.

B. Finite size scaling in ECRMs

In order to bridge the toy model with a small number of species and guilds with realistic ecological systems with large numbers of species and guilds, we scaled the parameters of the ECRM given different system sizes. As we increase the number of species N, we want to also increase both the number of guilds k and the number of species within each guild N/k. Hence, we set the number of guilds $k \propto \sqrt{N}$. The number of resources should also increase as $M \propto N$. Setting the probability of species i to have a non-zero intake of its preferred resource as p_{in},

and the probability of species i to have a non-zero intake of its non-preferred resource as p_{out}, we can compute the expectation value of the average degree of each species in the effective species-species interaction due to resource utilization overlap, the expectation value of $(CC^{\intercal})_{ij}$, etc.

Case 1: species i and j belong to the same community. The probability of that there is a no link between two species is equal to the probability that there is no common resource between the two, which is

$$P(CC^{\intercal}_{ij} = 0) = \left(1 - p_{\text{in}}^2\right)^{M/k} \left(1 - p_{\text{out}}^2\right)^{M(1-1/k)}. \quad (16)$$

Case 2: species i and j do not belong to the same community. The probability that there is no link is

$$P(CC^{\intercal}_{ij} = 0) = (1 - p_{\text{in}} p_{\text{out}})^{2M/k} \left(1 - p_{\text{out}}^2\right)^{M(1-2/k)}. \quad (17)$$

Given those two cases, the average degree for each node is

$$d = \left(1 - (1 - p_{\text{in}}^2)^{M/k} (1 - p_{\text{out}}^2)^{M(1-1/k)}\right) \left(\frac{N}{k} - 1\right) + \left(1 - (1 - p_{\text{in}} p_{\text{out}})^{2M/k} (1 - p_{\text{out}}^2)^{M(1-2/k)}\right) N \left(1 - \frac{1}{k}\right). \quad (18)$$

For proper scaling, we want that, in the limit of large N, the average degree d converges to a constant value. The choice $p_{\text{in}} \propto N^{-1/2}$ and $p_{\text{out}} \propto N^{-1}$ satisfies this condition, by ensuring that the average degrees towards in-guild and out-of-guild species are both finite. Notice that this scaling results in a $1/N$ scaling for both the expectation value and the variance of elements of the $\mathbf{CC}^{\intercal}$ matrix.

C. Measure sequence distance in marine eukaryotic OTUs

To measure sequence distance, we first align the 18S eukaryotic rRNA sequences of the $N_{\text{sub}} = 31$ eukaryotic OTUs using the Multiple alignment program for amino acid or nucleotide sequences (MAFFT) [48]. Then, sequence distance is computed for each pair of the OTUs, using the built-in MATLAB function seqpdist, namely the Jukes-Cantor distance.

D. Statistical tests for binned pairwise metrics against index shuffled null model

For analyzing the structure in the marine eukaryotic OTU timeseries data, we conduct statistical tests for the binned pairwise metrics against the index shuffled null model. Specifically, we shuffle the index of species randomly and then compute the pairwise measurements. This null model preserves the set of all elements of the pairwise measures, but destroys any association with the species relationships.

The statistical test conducted in Fig. 7(b) checks whether the mean of the 8 pairwise measurements in the first bin are significantly larger than in the index shuffled randomization. We performed index shuffling 10^5 times. For each randomization, we computed the mean in the first bin. We computed the p-value as the proportion of shuffling experiments that yielded a larger mean in the first bin than the observed one.

Acknowledgments

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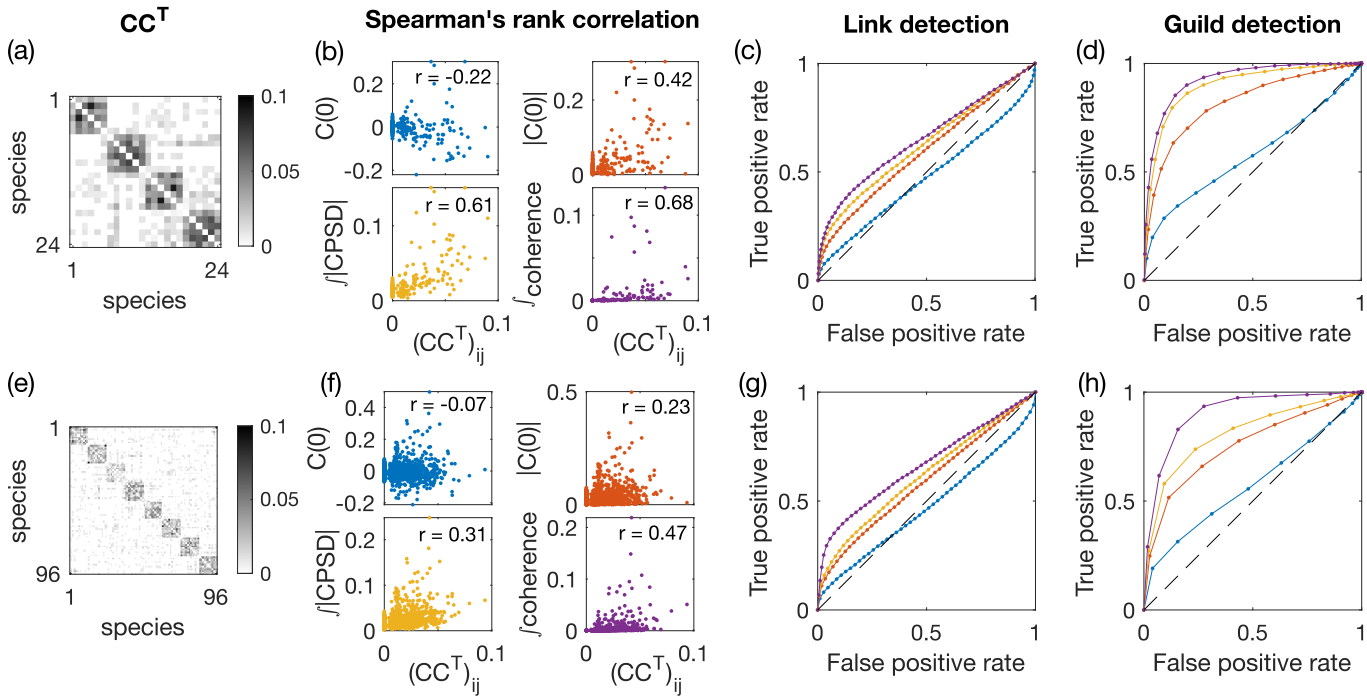

FIG. S1: **Pairwise observable analysis for the simulated ECRM ecosystem of different sizes.** Same as Fig. 5 but with $q = 0.4$.

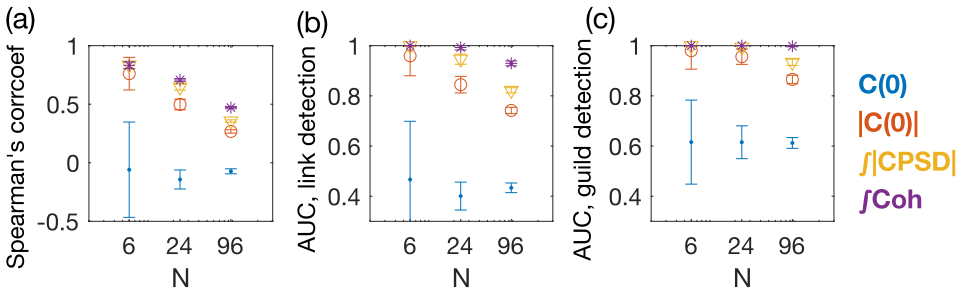

FIG. S2: **Coherence and CPSD outperforms equal-time correlation measures in recovering the resource-utilization overlap matrix $\mathbf{CC}^\intercal$ for all sizes of systems.** (a) Spearman's rank correlation coefficient between the four considered pairwise observables (equal time correlation $\mathbf{C}(0)$ and its absolute value $|\mathbf{C}(0)|$, the total magnitude of CPSD $\mathcal{P}$, and the total coherence $\mathcal{TC}$) and the elements of the $\mathbf{CC}^\intercal$ matrix, for three families of ECRM systems with $N = 6, 24, 96$ defined in Table 1. Error bars represent standard deviation across 100 random realizations of species abundances for systems with $N = 6$ and with $N = 24$ (10 random ECRM systems each with 10 random OU environmental drives with $\omega_\alpha = 1$), and across 10 random realizations of species abundances for systems with $N = 96$ (10 random ECRM systems each with 1 random OU environmental drive with $\omega_\alpha = 1$). (b) Area under curve (AUC) for link detection for the same systems as in (a). Each AUC is computed for the same ECRM system, averaged over the ROC of all 10 random OU drives. (c) AUC for guild detection after single linkage clustering for the same systems as in (a).

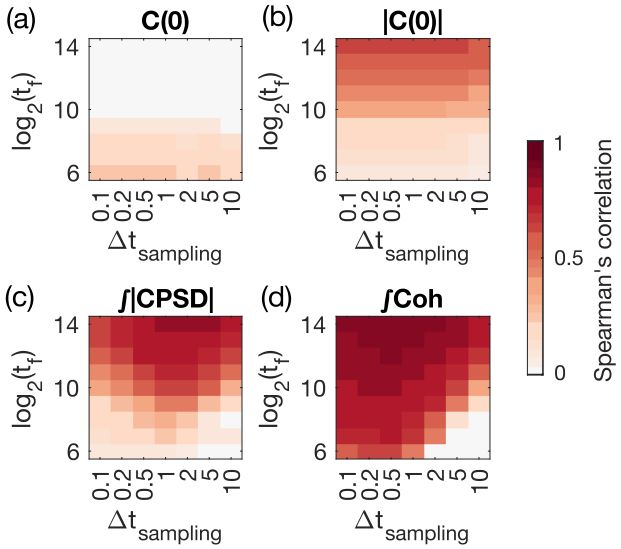

FIG. S3: **Influence of finite time-series duration and sampling rate on Spearman's correlation coefficient between the pairwise measures of species abundance and the resource utilization overlap matrix $\mathbf{CC}^{\intercal}$.** Spearman's correlation coefficient (colorbar) between elements of the $\mathbf{CC}^{\intercal}$ matrix and elements of (a) Equal-time correlation $\mathbf{C}(0)$, (b) its absolute value $|\mathbf{C}(0)|$, (c) the total absolute value of CPSD, and (d) the total coherence, as the function of sampling duration t_f and the sampling interval $\Delta t_{\text{sampling}}$. The ECRM is the same as the one considered in Fig. 3 with $N = 6$, with OU environmental drive with $\omega_\alpha = 1$ and guild-structure bias $q = 0.4$.

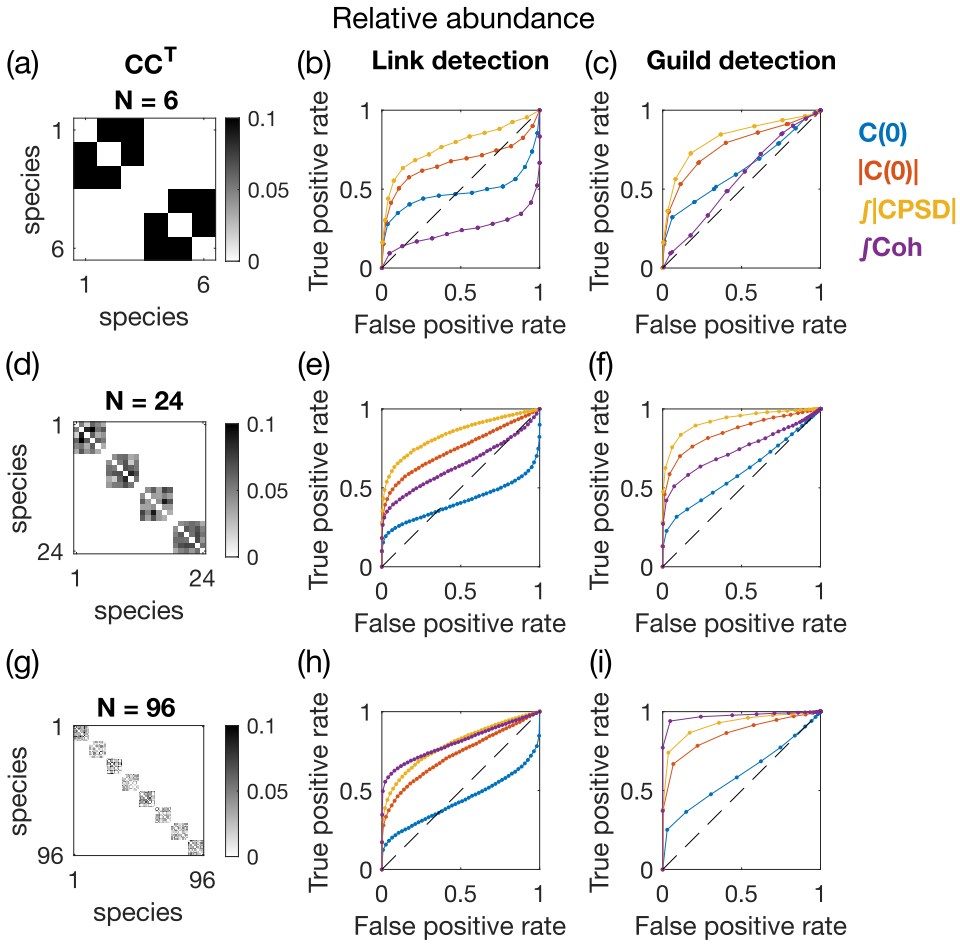

FIG. S4: **Link detection and guild detection of the resource utilization overlap matrix $\mathbf{CC}^\intercal$ using pairwise measurements of the relative abundance (instead of absolute abundance) of species concentration, for simulated ECRM ecosystems of different sizes** (Table 1), with guild-structure bias $q = 0.5$. (a) Effective resource-utilization matrix $\mathbf{CC}^\intercal$ with $N = 6$ species, $M = 30$ resources, $k = 2$ guilds, and $q = 0.5$. (b) ROC curve of link detection for the four pairwise observables. Legend for the colors is given next to panel (c). (d) Same as (c) but for guild detection, after performing single linkage clustering on the pairwise metrics with a tunable threshold. (e-h) Same as (a-d) but for $N = 24$, $M = 120$, and $k = 4$. (i-l) Same as (a-d) but for $N = 96$, $M = 480$, and $k = 8$. For all ECRMs, the environment is driven by OU processes with the intrinsic timescale set to $\omega_\alpha = 1$. For all system sizes, the total duration of the simulated trajectory is set to $t_f = 20000$, and the sampling timestep is set to $\Delta t_{\text{sampling}} = 1$.

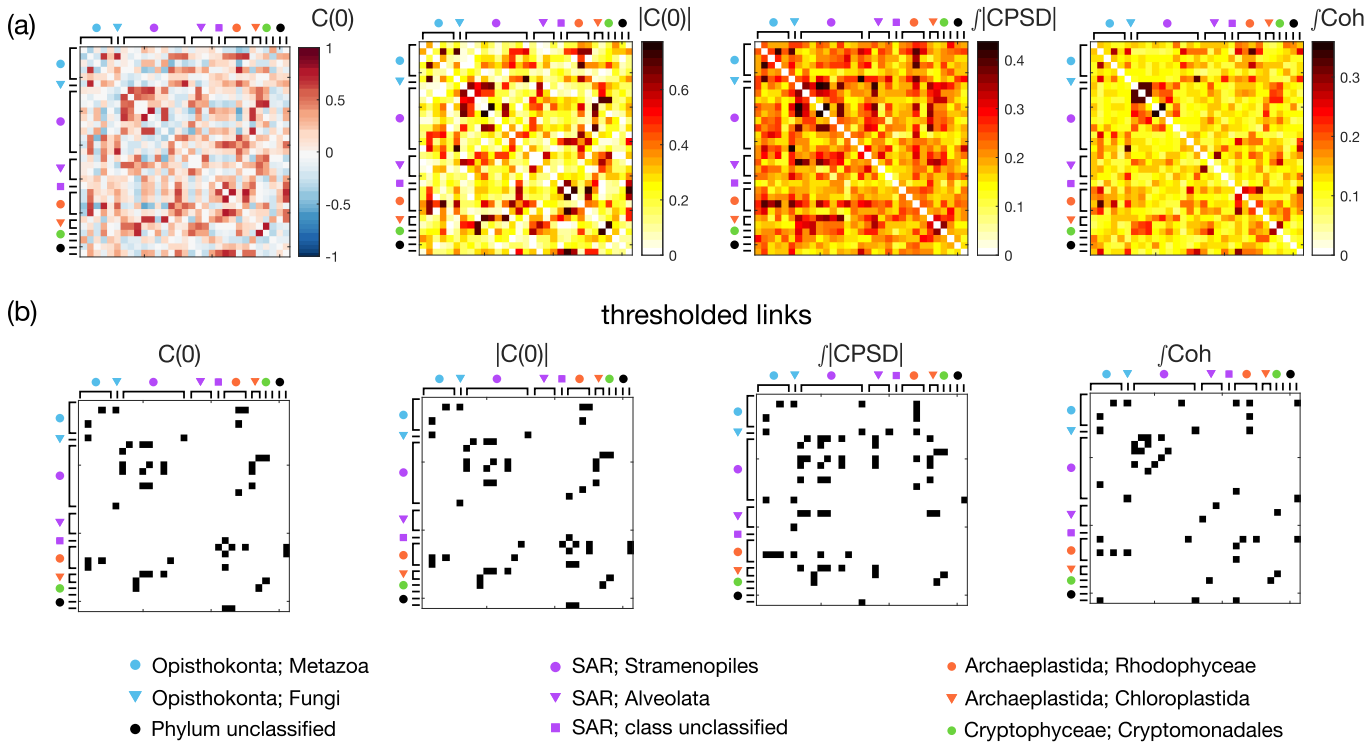

FIG. S5: **Pairwise measurements of the 93-day time series of relative abundance of eukaryotic OTUs in the Martin-Platero et al. coastal plankton dataset** (Fig. 7, data from [22], downsampled to $N = 31$). (a) Equal-time correlation $\mathbf{C}(0)$ and its absolute value $|\mathbf{C}(0)|$, the total magnitude of CPSD, and the total coherence of the time-series of relative abundance of marine eukaryotic OTUs ($N = 31$). The phylum and the class of each OTU is indicated by an unique color and shape (given in legend at bottom). (b) The adjacency matrix formed by thresholding the pairwise measurements in panel a to form $k = 13$ clusters (as in Fig. 7c and described in text). Black indicates a link, while white indicates no link.